

MONTE CARLO SIMULATION OF SOME DYNAMICAL ASPECTS OF DROP FORMATION

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Abstract

In this work we present some results from computer simulations of dynamical aspects of drop formation in a leaky faucet. Our results, which agree very well with the experiments, suggest that only a few elements, at the microscopic level, would be necessary to describe the most important features of this system. We were able to set all parameters of the model in terms of real ones. This is an additional advantage with respect to previous theoretical works.

Keywords: *Ising Model, Leaky Faucet, Monte Carlo Simulations*

1 Introduction

Many experiments [1-6] have confirmed that the dripping faucet, in spite of being a very simple system, presents complex behavior (chaos, Hopf bifurcations, long range anti-correlations, hysteresis, intermittence,...). Some years ago, a phenomenological macroscopic model was introduced [5] to explain the dynamical properties of this system based in the time interval between two drops. It was proposed that the drop oscillates like a mass-spring system, and the equation which represents it is given by

$$\frac{d}{dt} \left(m \frac{dy}{dt} \right) = mg - ky - b \frac{dy}{dt} \quad (1)$$

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where m is the mass of the forming drop, y is its position and g , k and b are constant parameters. This model reproduces some return maps similar to experimental ones, but it cannot give any information about, for instance, the drop shape and, in addition, the parameters could not easily be compared to the experimental ones. From a stochastic 2D boolean microscopic model in a square lattice, originally applied to determine the shape of a drop on the wall [7], some dynamical aspects of a growing drop were reproduced recently [8, 9]. These findings suggest that it is possible to obtain informations about the time series and drop shapes as a dynamical process. Besides this, other applications of lattice models to simulate macroscopic flow have been shown to be very useful. Some examples are the FHP cellular automata, which approximate the Navier-Stokes equations [10], and the study of mechanisms of fluid spreading with Ising model simulations [11].

In a recent experimental paper [12], two dimensional images of growing drops were obtained and studied by image processing techniques. In this work we show that from these studies, we succeeded in relating the computational parameters of the stochastic model [8, 9] to the real ones. We also discuss some morphological features of the drop formation similar to the ones exhibited in laboratory.

The main advantage of this lattice model in comparison with the differential-equation approach is that we can obtain information about the shape and, also, about time series with a large number of drops without huge efforts. However, in this work, we did not perform any smoothing of the drop surface because we are just interested in studying a model which displays the same dynamical behavior of real drops. It could be easily done if we are interested in the static shape of drops in a dripping faucet.

This paper is organized as follows: in sec. 2 we explain some features of the original model [8, 9] and the modifications needed to simulate wider faucets. In sec. 3 we present the results and conclusions will be discussed in sec. 4.

2 The Model

As in the original model [7, 8], we deal with a square lattice where the state of each site can be represented by Ising variables $\sigma = \pm 1$, where $+1$ means the fluid and -1 the air. In order to define the dynamics we introduced a hamiltonian function

$$\mathcal{H} = - \sum_{nn} \sigma_i \sigma_j - \sum_{nnn} \sigma_i \sigma_j - \sum_j h_j \sum_{row\ j} \sigma_i \quad (2)$$

where the first summation is over the nearest neighbors, and the second one is over the next-nearest neighbors. These terms play the role of both the molecular attraction and surface tension effects. The third summation refers to the presence of an external potential (gravity in the real system) varying linearly with the height, i.e., $h_j = g \cdot j$, where g is a constant and $j = 1 \dots V$, V is the vertical lattice size. A spin-flip Monte Carlo dynamics is imposed and it is performed by

Kawasaki trials (pair updates) imposing mass conservation. This is made choosing at random one element (air) in the external boundary and another one in the inner boundary of the drop (fluid). The flip of both elements do not change the mass but it can cause a variation of the energy as defined in equation (2). Hereafter, we call “relaxation” each pair update.

In the original implementation [8], there are W elements of fluid in the center of the first row of the lattice, representing the width of the faucet. There, the injection of fluid takes place, from the faucet into the drop, moving the drop one row down without changing its current shape. Here we choose a different approach. We inject F elements on the outer boundary, and relax the drop $N \times F$ times; i.e, $N \times F$ pair updates are made. In this way the drop movement will be governed only by the Hamiltonian \mathcal{H} . Time is defined proportional to the number of injections, and it is independent of the drop perimeter, other difference concerning the original model. This will allow us to compare drops at different regimes of flux. Then we can keep the “faucet width” (W) as constant changing only the flux (F) of fluid into the system to compare with the experimental data.

A fundamental modification refers to the way we can determine when the drop is disconnected from the top. Previously a burning algorithm was used, spending much computer time. Since we are working with large drops the disconnection is determined simply by searching for the existence of an empty row (at which all spins are zero) on the lattice, followed by a non empty row (that has at least one non-zero spin) at each drop relaxation. By a visual inspection we observe that inclined disconnections was not obtained (we consider only the zero temperature).

As we intend to show below, these modifications were important in order to relate the artificial parameters to the real ones.

3 Results

Our typical system size is a 128×460 square lattice (our 32 bit computer stores a 4×460 array, using 7360 bytes). This lattice size is approximately 12 times bigger than previous ones. We carried out our simulations on 486DX4 100Mhz microcomputers with 8 MB of memory. The code was compiled with GNU C using LIBGRX for graphics[14]. The CPU time is strongly dependent of the flux (as in the experiments, the smaller the flux, the larger the time required for a drop to disconnect from the faucet). In a typical run a time series of 500 drops ($W = 40$, $F = 5$) can be obtained after one hour.

We consider sets with 500 drops and $g = 0.1$, $N = 150$ and $W = 40$. The 100 initial drops in each set were discarded to avoid transient effects. All our results will be compared with the experimental ones[12], where two-dimensional images of growing drops are reported.

In Fig. (1) we show some steps of the drop formation for some values of F

(flux) to be compared with the real ones [12]. In the experiment the increasing volume of the drop is found to be proportional to time. The simulation presents the same qualitative behaviour, as shown in Fig. (2). Just like in ref 12, it was observed that the time evolution of the mean volume is

$$\langle V \rangle = V_0 + \langle \phi \rangle t \quad (3)$$

where $\langle \phi \rangle$ is the mean water flux, equivalent to our F . From this result we can verify that our redefinition of time is precise, whereas considering the number of relaxations to be proportional to the perimeter of the drop[9] do not reproduce this behavior.

We can verify the non-linear character of the drop formation looking at the center of mass height (y) as a function of time. This is presented in Fig. (3) for three successive drops, for two different values of F . As suggested in the experimental work, the drop presents a sort of “elastic behaviour” evident at beginning, while the center of mass height is still proportional to the time. After that the drop shows a “plastic deformation”, with a drastic change in the center of mass height. The current analogy is made in terms of the stress of some material under constant pressure, where after a well defined limit the material is deformed in a “plastic regime”. Another interesting aspect is that, as in the laboratory, the drops at higher flux regimes break down in a smaller time interval. This behaviour is also evident in Fig. 4, where we have the center of mass height (y) \times drop volume, to all drops on each set.

On Figs. 5 and 6, we choose one drop and show its area as a function of perimeter and perimeter over area as a function of time. These plots show that the simulated drops present the same relations between these variables which characterize the shape of the real drops. Once more the behaviour are qualitatively identical to the experimentally observed [12]. It is worth to note the time at neck formation, where also these curves change drastically their behaviors.

In summary, we have show that F is closely related to the flux and W is a fixed parameter which represents the faucet width. The parameter N (number of relaxations) is associated to the way the fluid relaxes or, in physical terms, its viscosity. Small values of N are associated with small viscosities. Now we will comment about the role played by the parameter g . In the previous work[5, 8, 9], different attractors have been reached with changes in g . But a simple dimensional analysis of \mathcal{H} shows that the last sum is the gravitational potential energy. If we imagine that each Ising variable σ_i represents a small element of volume dV , thus g can only be associated to the weight of that volume element. Since we have $weight = density \times gravity \times dV$, g can be associated to the fluid density or even the gravity.

4 Conclusions

We showed that a 2D Ising-like model can simulate the drop formation in a leaky faucet, both in the dynamical aspects and in the morphological ones as well. We relate all the simulation parameters with the real ones: F with flux, N with drop relaxation (viscosity), g with the weight of a volume element represented in the model by the Ising variables and W is associated to the width of the real faucets.

We could show that only a few elements, within a microscopic approach, may be enough to formulate a good theoretical model. Vibrations and instabilities in the drop surface do not seem important to complex behaviour of drops, from dripping faucets, since these ingredients are not taken into account in the present model. In a computational point of view, lattice methods are very fast and they can give us many additional informations as the ones from long time series, for example, which are very difficult to be obtained by the traditional theoretical methods, and of difficult control in the experiments.

It was presented in a recent paper[6] that time series from heartbeats present similar behaviour to that of leaky faucets. Therefore, we suggest that this lattice model could be used to provide more informations about the dynamics of the heart. Another immediate application is to generate long temporal series and to study the capacity of the chaotic prevision method applied to this complex regime. Works along these lines are in progress.

5 Acknowledgments

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- [14] The source code is available at: <http://www.if.uff.br/~arlima>

Figure Captions

Fig. 1 - Some steps of one drop formation. The numbers at left are the values of F (flux) used in the simulation. We did not perform any average to smooth their boundaries and the interval between the frames are not the same.

Fig. 2 - Volume as function of time for the last drop in the sets with $F = 5$ (\diamond), $F = 20$ (\circ) and $F = 30$ (\bullet). The linear behavior shows that our definition is in agreement with the real one.

Fig. 3 - Center of mass height of three successive drops, as function of time, for two different values of F ($F = 20(\circ)$ and $F = 30(\bullet)$). We can see that in regime with a lower F the drops spend more time to break down, exactly as in the experiments.

Fig. 4 - Volume as function of the center of mass height to all drops in the sets with $F = 5$ (a), $F = 10$ (b) and $F = 20$ (c). Again, the simulation agrees with the experimental results, since an initially linear behaviour was found. The saturation region (corresponding to neck formation) is also observed.

Fig. 5 - Drop area vs perimeter. We present the results for only one drop at the set $F = 5$. Similar plots are found for all other drops.

Fig. 6 - Ratio drop perimeter/area as a function of time. We consider the same drop as in Fig. 5 for the $F = 5$ set.

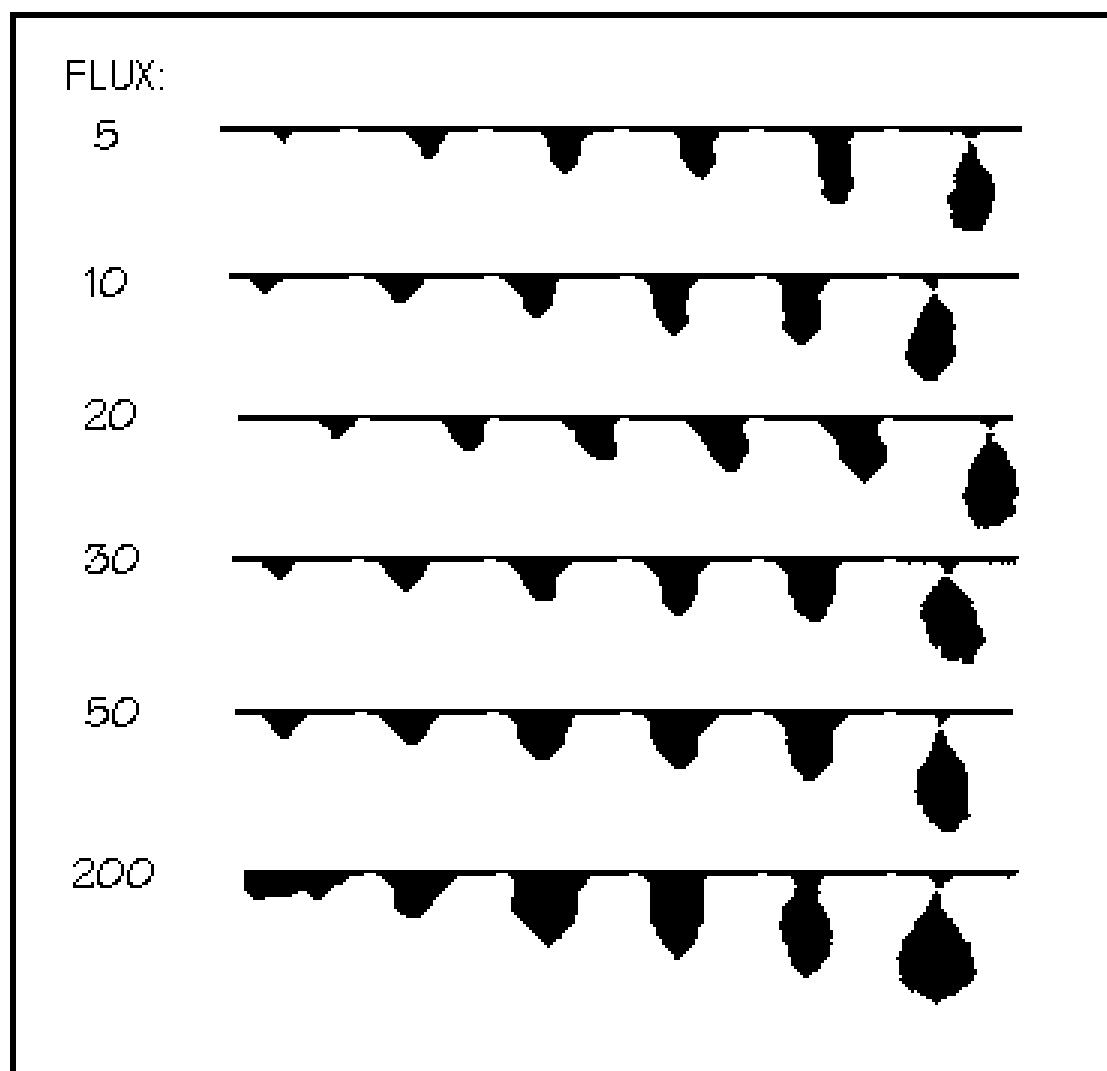


Figure 1 - A.R. de Lima, T.J.P. Penna and P.M.C. de Oliveira

Figure 2 - A.R. de Lima, T.J.P. Penna and P.M.C. de Oliveira

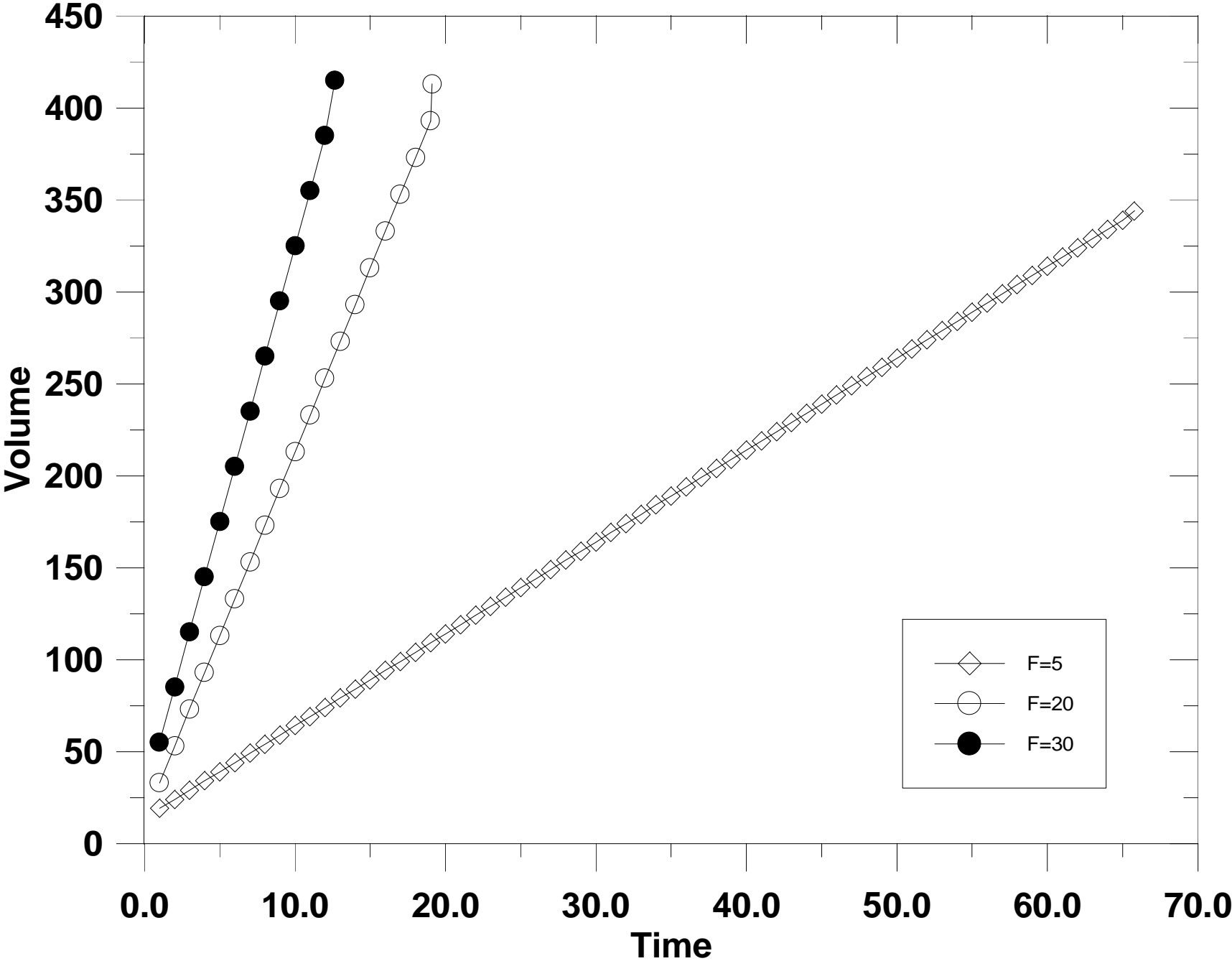
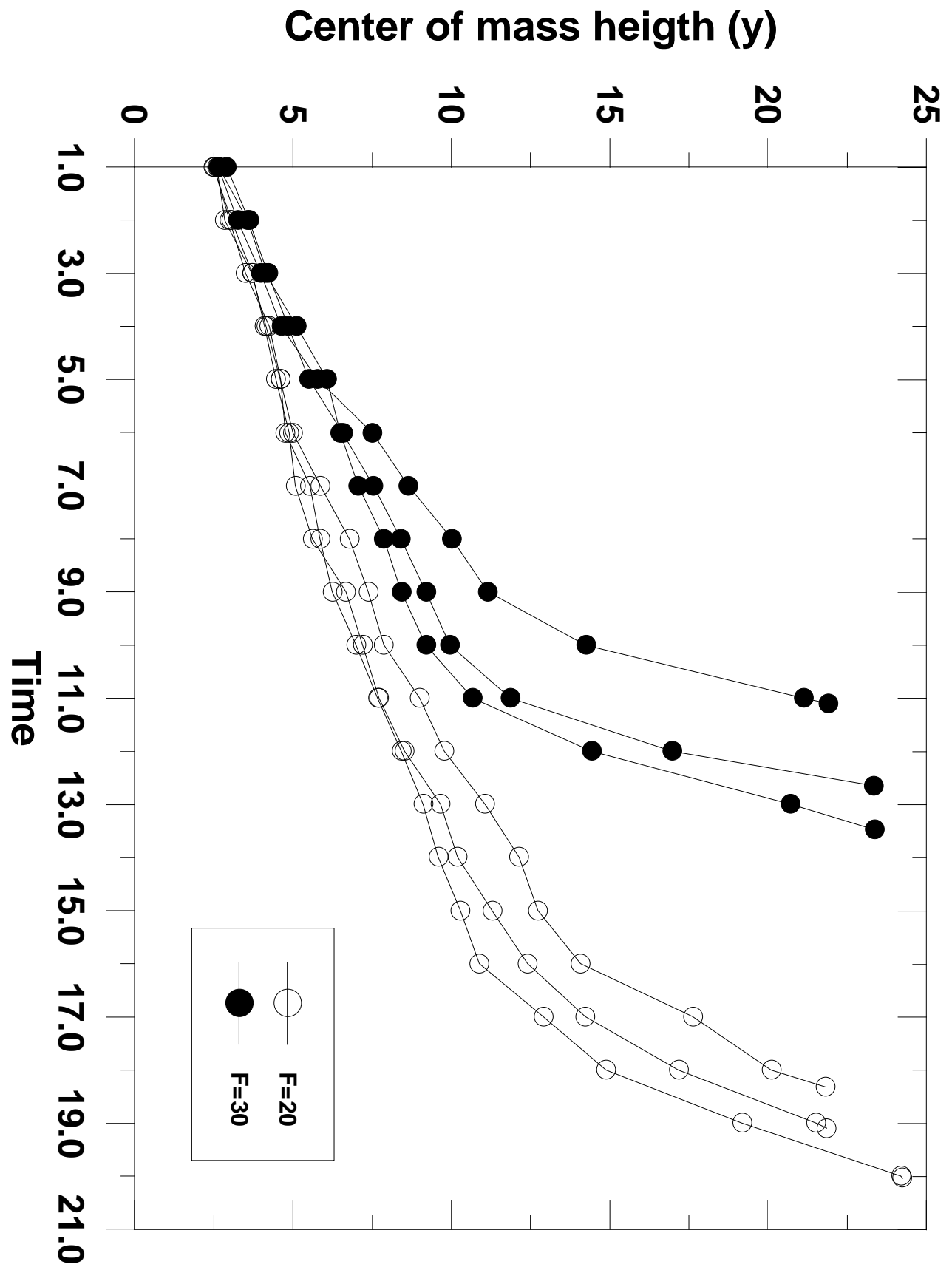


Figure 3 - A.R.de Lima, T.J.P. Penna and P.M.C. de Oliveira



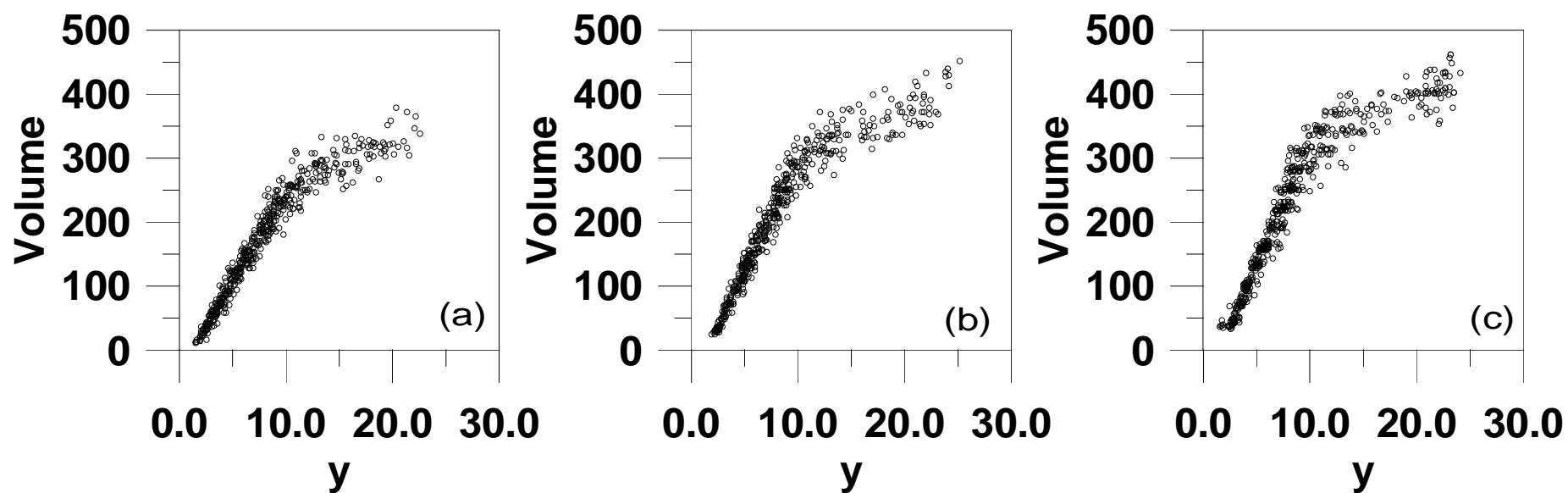


Figure 4 - A.R.de Lima, T.J.P. Penna and P.M.C. de Oliveira

Figure 5 - A.R. de Lima. T.J.P. Penna and P.M.C. de Oliveira

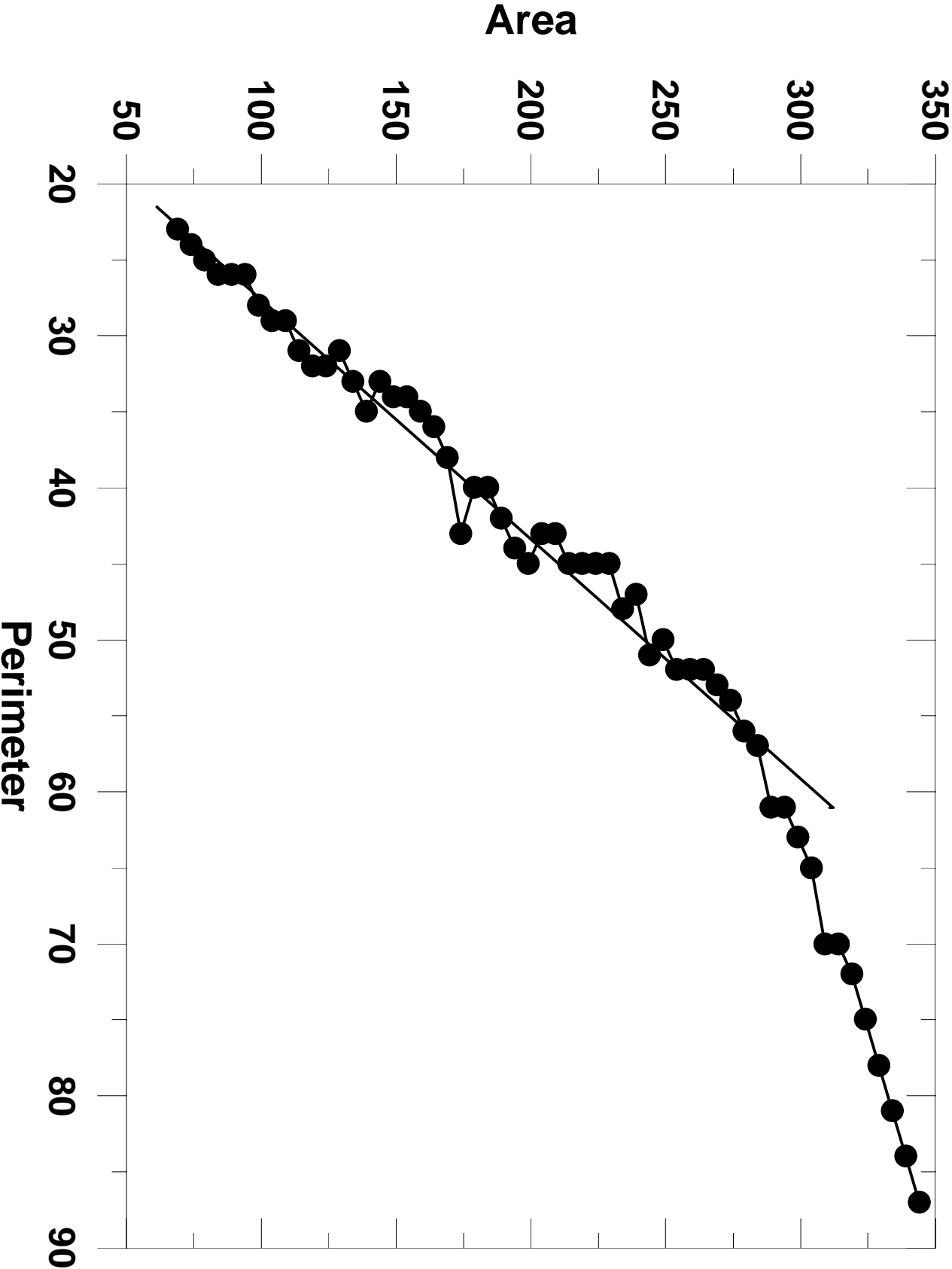


Figure 6 - A.R. de Lima, T.J.P. Penna and P.M.C. de Oliveira

